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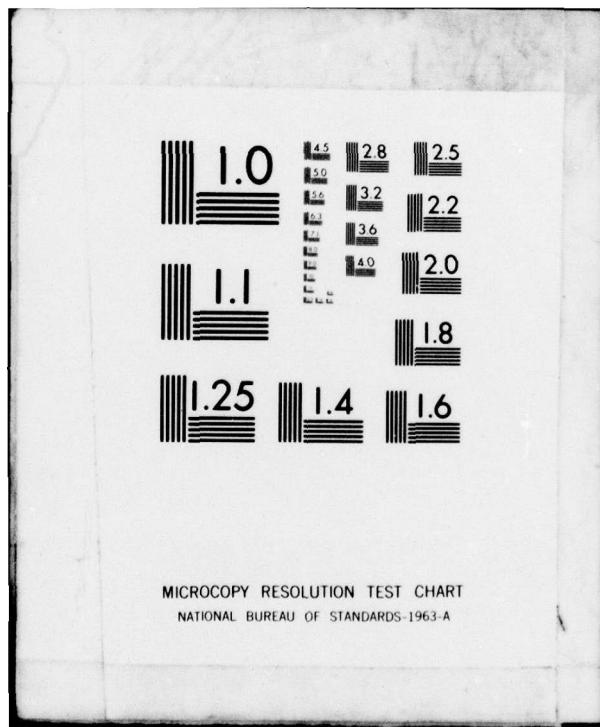
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H. D. Brody

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<table style="width: 100%; border-collapse: collapse;"> <tr> <td style="width: 33%;">Solidification</td> <td style="width: 33%;">Continuous casting</td> <td style="width: 33%;">NITINOL</td> </tr> <tr> <td>Computer simulation</td> <td>Welding</td> <td>Superalloys</td> </tr> <tr> <td>Process modelling</td> <td>Peritectics</td> <td>Simulation</td> </tr> </table>			Solidification	Continuous casting	NITINOL	Computer simulation	Welding	Superalloys	Process modelling	Peritectics	Simulation
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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)											
<p style="margin-left: 20px;">Status of projects related to directional solidification of peritectics, segregation of nickel base superalloys, and casting of NITINOL are summarized. A paper is included which describes work done and needed on modelling of casting processes.</p>											

STRUCTURE AND PROPERTIES OF CAST ALLOYS

ONR Contract N00014-75-C-0800

Technical Summary

Work since the last technical report has concentrated on two areas: understanding segregation phenomena in nickel base superalloys and directional solidification of peritectic alloys. Additionally, some work has been aimed at preparing NITINOL alloys. An attached paper¹ reviews work on modelling of casting processes including pulsed arc welding².

Directional Solidification of Peritectic Alloys

Controlled directional solidification of peritectics led to surprising results. In Pb-Bi and Sn-Cd model systems, it was found that moderate values of the ratio of thermal gradient to growth rate, G/R, led to aligned two phase composites; while high values of G/R led to supersaturated single phase alloys³⁻⁵. A theory was developed to relate growth conditions to microstructures in these systems. Extensive electron microprobe measurements of Sn - Cd samples have been taken in the region of the three phase cellular interface ($\epsilon + \delta + L$), the planar δ/L interface, and banding associated with breakdown of the planar δ structure. Agreement of the theory developed with the electron microprobe results can be obtained only if the published phase diagram for Sn - Cd is incorrect. A check on the pertinent part of the Sn - Cd phase diagram will be made.

Planned work includes thermal measurement of the interface temperatures in the Sn - Cd system plus extension of the experimental work to systems with higher peritectic reaction temperatures. The experiments on the new system will be used to determine if the observations and theory developed in the low temperature systems are applicable to higher temperature systems.

Segregation in Nickel Base Superalloys

Studies of segregation in nickel base superalloys indicated (1) that extent of microsegregation varied with cooling rate in the range of 10^{-2} to 10^2 °C/sec. and (2) that hafnium additions accentuate the macrosegregation associated with changes in cross section.^{6,7}. In order to gain a fundamental basis for understanding the aforementioned segregation behavior, a procedure was developed for determining the distribution coefficient for the key substitutional elements, measurements of the liquid densities of several alloys were made to develop the relation of liquid density to alloy composition and temperature, and theories of micro- and macrosegregation have been applied to the solidification of these ten component alloys.

The distribution coefficient for hafnium is much less than one and hafnium promotes eutectic formation. In hafnium modified alloys, diffusion in the solid dendrites during freezing appears to be retarded leading to near maximum eutectic formation during freezing. There is significant redistribution of solute elements during the freezing of alloys with no hafnium additions and the eutectic formed is closer to the equilibrium prediction.

The density of the last liquid to freeze in alloys without hafnium is less than the nominal liquid density. The addition of hafnium, which concentrates in the liquid, decreases the difference in densities. However, the major influence of hafnium on the macrosegregation tendencies of nickel base superalloys stems from its low distribution coefficient and its eutectic forming character. The details of this investigation are the subject of the next technical report.

NITINOL Casting

In cooperation with the Naval Surface Weapons Systems Laboratory, we have been developing research lot procedures for preparing NITINOL alloys. These alloys are made available for research purposes. NITINOL alloys have been prepared in approximately one pound and ten pound lots.

The smaller quantities are formed by arc melting and drop casting. First buttons of titanium, from sponge, and nickel, from electrolytic nickel, are arc melting under about one-third atmosphere of argon. Then the buttons are cut and weighed to the nearest 0.0005 grams to prepare the NITINOL charge. The pieces are arc melted into a button, flipped and melted again. Then the button is placed in a hearth with a central hole. The alloy is melted again and allowed to drop through the hearth into split copper molds.

The larger lots are formed by induction melting. First the nickel shot and titanium sponge in the desired proportions are partially fused to make 0.5 - 1 pound compacts to fit the induction melting crucible. The crucible pouring lip and molds are all made of machined graphite. A starter slice of NITINOL is placed in the bottom of the crucible and the partially fused compacts of titanium sponge and nickel shot are stacked above. The melts are made under a vacuum of 1 - 10 microns and poured into unheated, risered molds.

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SIMULATION OF SOLIDIFICATION PROCESSES

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ABSTRACT

Process modelling has been applied to analysis of solidification operations and phenomena for the purpose of increasing basic understanding of the processes, to develop procedures for design and control, CAD/CAM, and to aid in automation. Simulation of solidification is illustrated by models of the development of microsegregation, heat flow in pulsed arc welding, heat flow in large ingots/castings, heat flow and stress in continuous casting, designing castings for mechanical properties, and automatic generation of patterns for shaped castings. Areas for continued research and development are suggested for these areas of casting interest.

A solidification step is included in the processing of most of the items made from metals and alloys. The cast structure (porosity, tears, inclusion size and distribution, dendrite morphology, grain size, microsegregation and macrosegregation) produced in shaped castings is modified only slightly before the part is put in service. For ingots, continuously cast slabs, billets, and rods, incrementally solidified ingots (ESR, VAR), and atomized powder, the cast structure is modified by thermomechanical processing. However the influence of the cast structure carries to the final product. Further, the cast structure influences the success of thermomechanical processing and overall productivity. In welding, solidification within and adjacent to the fusion zone is critical to the quality of welded components.

The modelling of solidification processes to date has been directed, primarily, to gaining a better understanding of the influence on cast structure by the casting parameters and alloy properties. Process modelling will be increasing in importance for process design (CAD/CAM) and automation.

In solidification of alloys the models that have been developed are concerned with

- ' the phase transformation, i.e. morphology and kinetics.
- ' the transfer of heat by all modes within the alloy, within the mold, and to the environment
- ' fluid flow in the bulk liquid, in the mushy zone (region where solid and liquid coexist), and in the mold
- ' mass transfer by diffusion in liquid and solid phases and by bulk flow in the liquid
- ' stress build up and deformation by thermoelastic, plastic and creep deformations.

Simulation of alloy solidification for research purposes has been combined with experimentation to upgrade our understanding of casting practice from a near black art two decades ago. Solidification principles have been developed in a step-by-step progression. Simulations have been tried based on existing principles and judgment. The predictions of the simulations have been tested by critical experimentation. Often it became clear that important factors had been ignored or given too little weight. Measurements were made to characterize behavior and/or determine material properties or operating parameters. Then, improved models were developed based on the upgraded principles and expanded data base to start another cycle of simulation and experimentation. Progress made supports continued application of the two pronged approach to increasing definition of solidification principles and the understanding of solidification behavior in complex casting processes and multicomponent alloys.

A model is limited in its applicability by the validity of the assumptions on which it is based and the accuracy of the input data. Once a model is developed it is essential that it be validated. This may be a difficult task. The complexity of the process being simulated might rule out the use of analytical expressions to check the numerical techniques; and

it may be prohibitively expensive or difficult to make direct measurements on the process. It should be pointed out that in not a few cases the availability of a model has spurred the collection of data that proved surprisingly useful on its own. A model will be extrapolated beyond the region where it has been validated. The success of the extrapolation will depend on the care and insight that go into model building and the effort that is expended in validating the model.

The use of process modelling for process control and automation has been growing slowly, but application now promises to expand manifold. As a result solidification processes can or will be run more reliably, decisions based on computations made more quickly, documentation and record searching more encompassing and efficient. The processes and design of processes will be less dependent on the experience of a few key individuals. In short, application of computers will be based on process models and the control afforded will improve reliability and productivity.

Further, the utilization of computers for process simulation should provide a tool for utilizing more powerful design concepts. The designers' "black magic" or intuition will be put on a sounder base. Design principles that could not be carried further than "rules of thumb" or semiquantitative guidelines (e.g. Chvorinov's rule, Caine's curves, feeding distances^{1,2}) could be expanded to have bases in the principles of heat flow, fluid flow, mechanics, and metallurgical structure. Beyond designing castings to avoid gross shrinkage with a reasonable yield, castings could be designed to meet high mechanical property requirements.

Microsegregation

The study of microsegregation in the dendritic freezing of binary alloys provides a well-known feature of cast structures that results from the partitioning of solute between solid and liquid phases.¹ An initially homogeneous liquid will yield solid with a nonuniform distribution of solute on the scale of the dendrite arm spacing. The relative importance of liquid and solid diffusion in controlling solute redistribution during freezing was resolved by the two pronged approach.^{3,4} A model was developed by selecting a characteristic volume element and by making reasonable assumptions about the thermal condition, mass transport, and geometric character of dendritic freezing. The basis of the model is illustrated in Figures 1 and 2. A finite difference numerical analysis technique was used to compute the contribution of solute diffusion in the growing solid phase to reducing the extent of microsegregation.

The model, which was intentionally kept simple, was applied to a simple binary eutectic system, i.e., aluminum-copper alloys; and unexpectedly, the model indicated that

- ' There should be a measurable contribution from diffusion in the solid phase, i.e. limited solid diffusion.
- ' Microsegregation manifests itself by lowering the solidus temperature to the eutectic, by producing coring in the primary phase dendrites, and by producing or increasing the eutectic constituent.
- ' By inference, and also calculable by the model, when diffusion in the solid is limited, diffusion within the liquid of the volume element must be complete.
- ' The reduction in coring on cooling below the eutectic temperature is much less significant than during freezing.
- ' The extent of as cast microsegregation is not very sensitive to cooling rate for common casting processes.

The predictions of the model could be checked experimentally. The amount of eutectic had been measured for several copper contents previously, and the results followed the trends of the model.^{4,5} If solid diffusion during

freezing were significant, a change should occur in the composition of the center of the dendrite. The solidification of small samples was interrupted at different solid fractions and the copper content measured with an electron microprobe.⁴ Results confirmed the prediction of the model that the copper content at the centers of the dendrites increased during freezing. Additionally, thermal measurements confirmed the basic assumption of negligible undercooling at the dendrite tips.

Although the initial model was quite simple and the most important materials parameter, the diffusion coefficient, was not known very accurately, the model was instrumental in uncovering the factors that are key in determining the extent of microsegregation in a wide range of casting practice. The model has been modified since to determine and include the influence of different dendrite geometries,⁶ dendrite coarsening,⁷ systems with higher^{6,8,9} and lower^{7,10} solute diffusion coefficients than Cu in Al, grain structure,⁹ peritectic alloys,⁹ and selected ternary systems.⁶ Further the microsegregation model has been included as a basic component of the development of models of macrosegregation,¹¹ inclusion formation,¹² porosity,¹³ shrinkage,¹³ and heat flow in E.S.R.¹⁴ and D.C. casting.¹⁵⁻¹⁷

Further Research:

Microsegregation is not understood well enough for the analysis of many nagging industrial and developmental problems. Further modelling promises progress in understanding the principles and control of microsegregation, in particular in

- ' multicomponent systems where several components have limited diffusion in the solid during freezing
- ' newer/non-conventional freezing processes where undercoolings at dendrite tips may be a significant fraction of the total freezing range.

The data base of materials properties may be insufficient to allow accurate representation of material behavior and prediction of microsegregation in the cast structure. However, use of reasonable estimates of materials properties will demonstrate the trends that may be expected, indicate the range of casting conditions in which classes of behavior may be expected, and indicate which parameters are the ones that should be controlled.

Pulsed Arc Welding

A second example of the two pronged approach is current research directed at gaining a fundamental understanding of the relation between operating parameters, materials properties, and structure in the fusion zone for pulsed tungsten arc welding. A two-dimensional heat flow model,^{18,19} using finite difference techniques, has been developed to simulate the thermal conditions in pulsed arc welding of sheets. A moving arc is simulated, the power input is cycled as in the typical current cycle in Figure 3, heat is transported from the fusion zone by conduction, and may be lost to the surroundings by convection and radiation. Convective transfer in the liquid pool is simulated indirectly by multiplying the thermal conductivity by an arbitrary factor. Initially a factor of seven was selected based on previous experience with continuous casting.^{17,20} The model was checked for consistency with previous analyses which are applicable to continuous welding. Agreement between the numerical model and Wells²¹ equation for predicting the size of the fusion zone were good. Temperature distribution away from the fusion zone was in good agreement with Adams²² equation, note Figure 4. Analytical expressions were not available for either computation of temperature distributions in and near the fusion zone in continuous welding or temperature distribution and weld bead size in pulsed arc welding.

Sheets of Fe-26%Ni were welded systematically changing peak and background current (i_p and i_b), the ratio of peak to background duration (t_p/t_b), period (T), and travel speed (v). Thermocouples were inserted in selected welds. Thermal records of positions adjacent to the fusion zone in two pulsed arc welds are shown in Figure 5.

Comparison of initial predictions of the model and experimental measurement of the weld bead width indicated that the computed weld beads were too small. It was determined that good agreement could be obtained if the amount of convection simulated in the fusion zone were increased substantially by multiplying the thermal conductivity by a factor of 25 (substantially higher than the factor of seven used for continuous casting). Thus, the model indicated substantial fluid motion accompanies pulsed arc welding. Concurrently, metallographic evidence has pointed to the effect of fluid motion. Initial analysis of high speed movies of the fusion zone indicates a complex pattern of fluid motion. With the inclusion of increased convection in the model the predictions of growth rate and thermal gradient are in good agreement with experimental measurement.^{18,19}

Further Research:

The initial disagreement between the model and the experimental results pointed to the importance of fluid motion in pulsed welding processes and the need for

- ' further modelling of the interaction of the magnetic field of the pulsing arc, the thermal field, and the alloy characteristics
- ' detailed experimental investigation of the influence of intense fluid motion on the structure of cast metals under conditions of a steep thermal gradient.

Designing Large Steel Castings

The design of molds for large steel rolls is a definite example of a case where evaluation of alternate designs by computer simulation is much less expensive than industrial trials. One design criterion is to avoid regions likely to form gross shrinkage. This would require an analysis to predict isotherm movement (especially liquidus and solidus isotherms) for complex mold designs. The heat flow can be simulated by a two-dimensional finite difference analysis representing the general cylindrical symmetry of the mold design.²³ The mold design is different at the drag neck, the cope neck, and the roll body. Facing sands, metal chills, and external power input have been used to control heat flow in the mold. A major concern is determining the appropriate materials properties.

As example, simulating a mold design not used in practice, the position of the liquidus and solidus isotherms at a stage near the beginning and the end of freezing of a 130 cm. diameter roll are shown in Figures 6 and 7. It is clear from these diagrams that the hypothetical mold design indicated would lead to gross shrinkage in the roll body below the cope neck.

Further Research:

Such heat flow analyses for large static ingots and castings have become common. The major need is to obtain the relevant thermal properties of mold materials, alloys, and the effect of interface resistance. Of concern for further study would be the analysis of macrosegregation and stress build up in these large cast bodies. One factor with influence on macrosegregation and on the macrostructure is convection in the liquid and mushy zones. More modelling and experimental characterization is needed on the fluid motion.

Control of Continuous Casting

For D.C. (direct chill) continuous casting one of the concerns is the formation of radial cracks near the center. Modelling of the heat transfer and build up of thermal stresses offers the possibility of understanding the interaction of alloy and casting parameters that lead to cracking, defining parameters to be controlled in order to reduce cracking, and a way of evaluating the effect of changes in operating parameters and caster design. A side benefit has come from the need to supply input data to the models. The measurement of operating parameters and materials properties has uncovered factors in current practice not realized previously.

The model¹⁴⁻¹⁶ of steady state operation of D.C. casting of cylindrical ingots is based on finite element methods of numerical analysis for both heat flow and thermal stress. The heat flow analysis is two dimensional (radial and axial), accounts for the motion of the ingot, has varied boundary conditions for the refractory header, mold, and various water cooling regions. In the mold the formation of an air gap may be taken into account. For much of aluminum casting practice heat flow in radial and axial directions are comparable. The thermal stress analysis is three dimensional, taking into account thermoelastic, plastic, and creep deformations. For convenience in interpretation the stresses may be normalized by dividing the absolute stress in a region by the yield stress of the alloy at that temperature.

Examples of the results of the model are shown in Figures 8 through 10. Figure 8 indicates the steady state position of liquidus and solidus isotherms for ingots of different diameters. Figure 9 indicates the distribution of normalized stresses in the larger of the D.C. ingots included in Figure 8.

Figure 10 illustrates the use of the model to determine the effect of reduced cooling for a controlled length below the mold. The maximum normalized stress in the central region of the ingot near the solidus isotherm, which is related to the formation of radial cracks, is shown in Figure 10 as a function of the reduced cooling length and the heat transfer coefficient in the reduced cooling zone. The aim would be to minimize the maximum normalized stress in this region. On the other hand, the effect of these casting parameters on surface stress and residual stress must be considered as well.

Further Research:

The modelling of continuous casting has substantial potential in process control. In continuous casting there are a variety of parameters that can be controlled and changed during operation. Because of the large investment in capital equipment, it is advantageous to know well the character of the operation and to be able to simulate the results of design or operating modifications. Continued development of these models would benefit from

- ' modelling of transient conditions
- ' better characterization of the mechanical properties of alloys at high temperatures
- ' characterization and modelling of the effect of fluid flow
- ' further collection of thermal properties of mold materials and alloys and heat transfer coefficients
- ' development of fracture criteria suitable to casting processes, e.g. hot tearing models.

Designing to Reach Critical Properties

The extension of heat flow modelling beyond analyses of macroscopic defects, shrinkage, pipe, cracking, to the area of designing so as to control cast microstructure and as a result to control strength and ductility properties of the casting is within the scope of present understanding

and hardware availability. The illustrations of the results of heat flow analyses so far have been restricted to indicating positions and progress of key isotherms. More detailed analysis of heat flow would allow calculation of localized cooling rates, \dot{t} , thermal gradients, G, and isotherm advance rates, R. Making allowances for melting and teeming practice, variations in chemistry, fluid motion, and the effect of subsequent thermomechanical processing, G, R, and \dot{t} can be related to the main features of cast structure and through them to the properties of the final product.

One example of the relation of the local thermal conditions to a microstructural feature has been developed for carbide (MC) morphology in nickel base superalloys,²⁴ as shown in Figure 11. Similar maps relating microstructure to heat flow parameters could be obtained for other features of cast structures, including dendrite spacing, microporosity, average inclusion and other particle diameter, and microsegregation. These features, in turn, have a strong influence on mechanical properties. Although the relations have been shown over and over again, they have not been placed on a generalized form that is suitable for process design. The early work of Passmore, et al.²⁵ illustrated in Figure 12 demonstrates the ability to control cast properties by controlling heat flow and microstructure. While their results were not reported in the fashion desired for design, it is reasonable to think that the data could have been collected and reported as in Figure 13. Coupling this type of map with a heat flow simulation would allow computer aided design of casting processes with final properties as a design criterion.

Further Research:

The critical work needed here is a demonstration of the concept. Because of this goal and others it would be useful to develop simulation techniques that could handle an arbitrary three-dimensional geometry and arbitrary boundary conditions. Such modelling might be based on group technology.

Pattern Construction

The design and construction of a pattern for a shaped casting is a key step that is often dependent for its performance on an individual with a background of intuitive experience.² The design procedure requires judicious application of rules of thumb, tedious calculations, and careful drafting. The pattern must be designed to allow draft for drawing the pattern, enlarged dimensions to allow for shrinkage, cores and core prints for forming internal cavities in the part, risers and chills to feed shrinkage and promote progressive freezing, and a gating system for filling the mold cavity. This is an example of where computer software can be designed to do some or all of these steps automatically in assistance of the designers.

The automatic transfer of the geometric description of the required cast part to a computer console will be possible in the near future. The calculation of draft and shrinkage allowance can be made to be automatic. The designer could specify the position of risers and their dimensions or use computer simulation to aid in making the rigging decisions. Also, the designer could designate the gating system with or without the aid of computer simulation. Then, the designer can prepare an N/C tape on the computer. For record keeping purposes drawings of the pattern design can be made automatically. The pattern itself can be accurately machined using the N/C tape generated on the computer.

Summary

A few of many possible examples have been presented to indicate the use of process modelling to aid in the understanding, design, control and automation of solidification processes. When process modelling advances are coupled with the present and promised advances in computer hardware and software and the development of specialized instrumentation, it

is anticipated that automation plus CAD/CAM will mushroom in casting processes of all scales.

It should be emphasized however that simulation and CAD/CAM would not remove the need for human input. Interaction of the engineer with the CAD/CAM systems would be essential; and through the interaction the engineer will be more efficient and will be able to consider and test factors previously out of the scope of practicality. Efficiency will result from the ability to make necessary calculations rapidly and accurately with the results of the design placed reliably and consistently into a useable form. The design generated by the CAD/CAM process can be saved to accurately record the procedures followed, thus facilitating confirmation of results and post mortem analysis. By present methods an inferior design might be accepted because of impatience or an unwillingness to invest effort and resources in further trial and error procedure. The CAD/CAM approach should yield a good result in the first production run. Alternate design concepts could be evaluated on the interactive screen and the best option selected.

Beyond automating and facilitating present practice, simulation affords a more powerful tool for expanding the creativity of individuals. It allows the application of design and control procedures based on complex simulations. Also, it fosters new ideas and understanding by giving the researcher an added tool.

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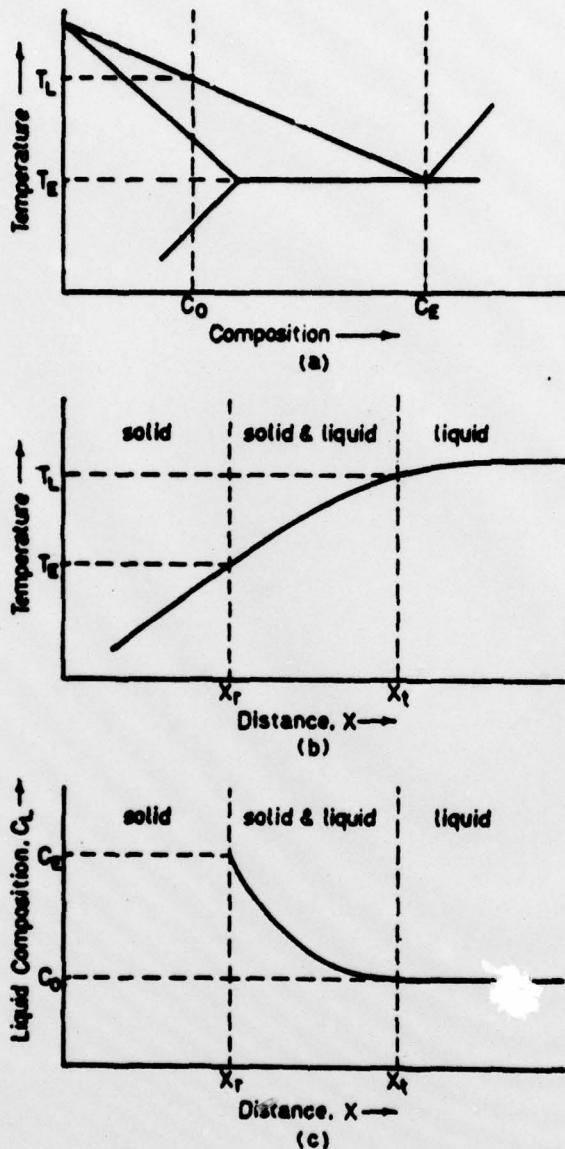


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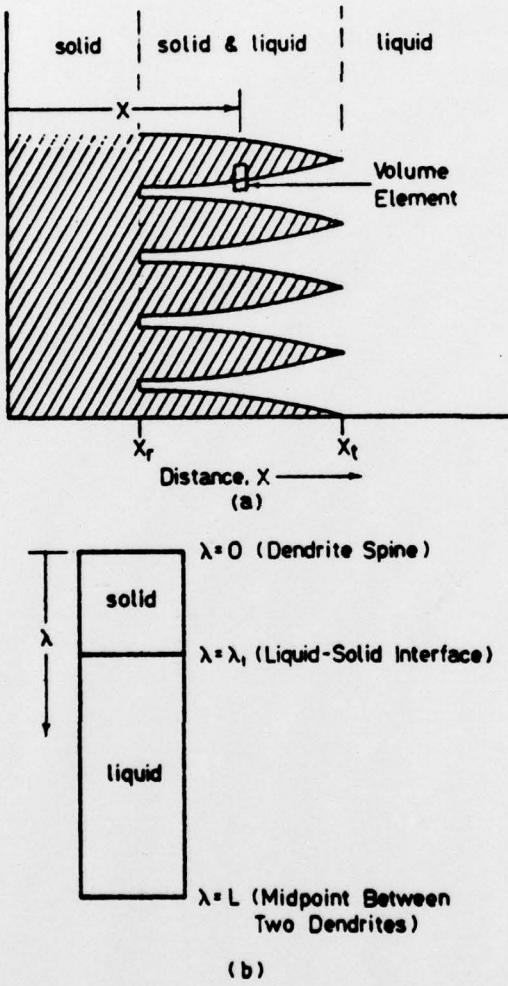


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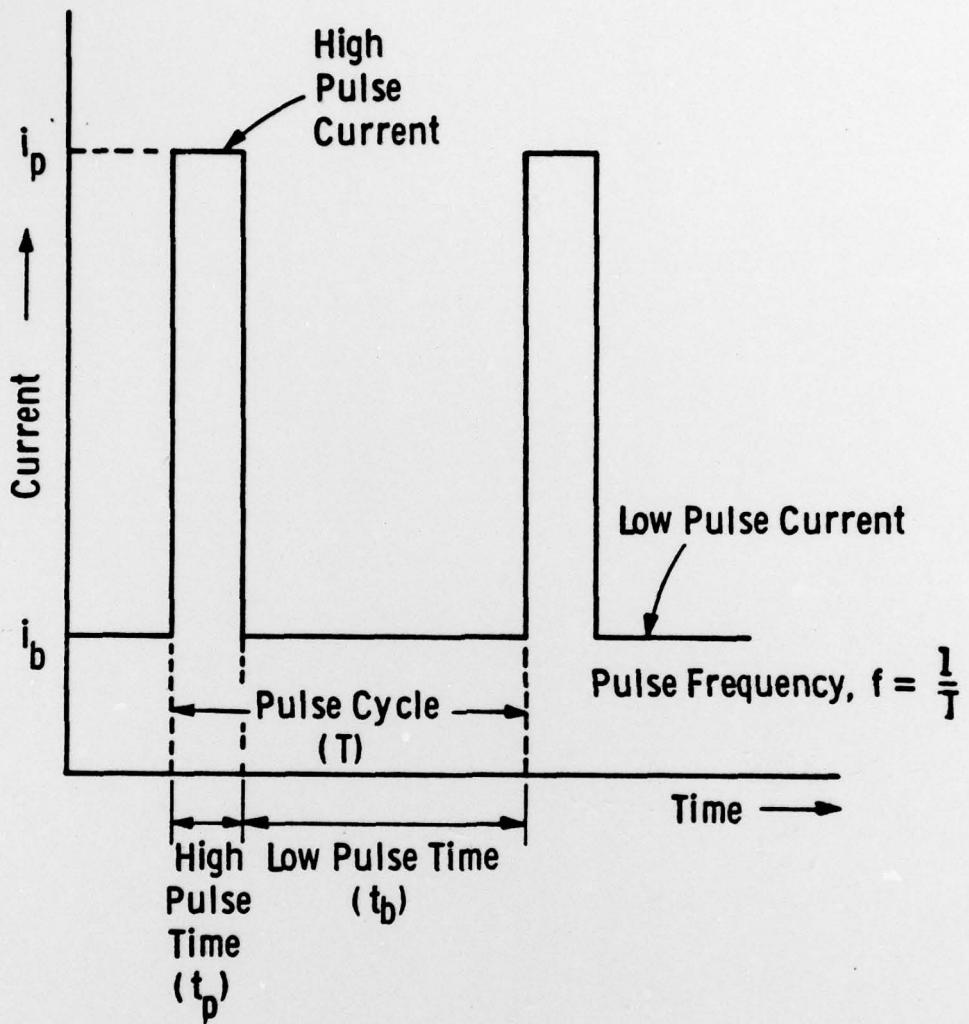


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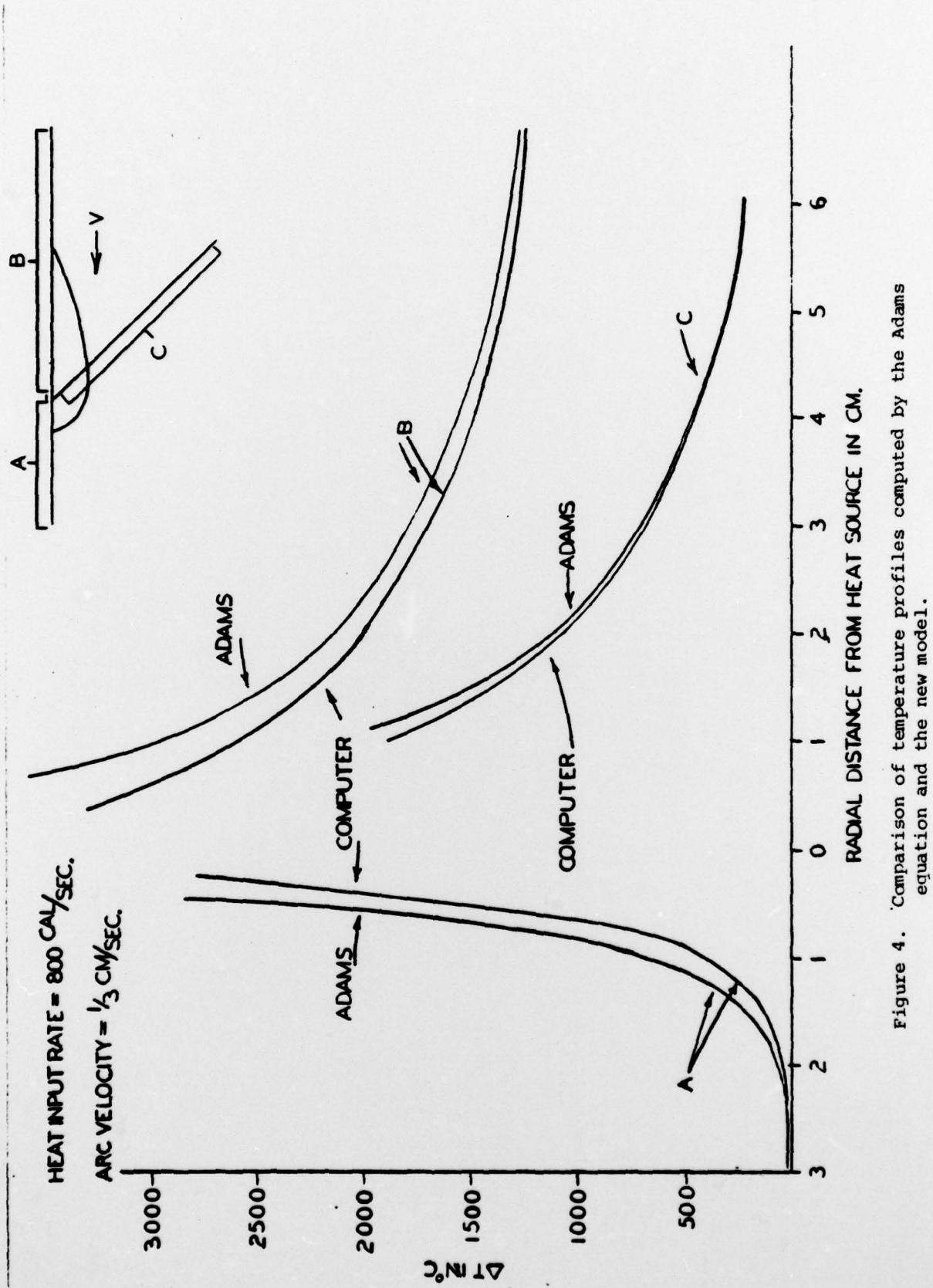


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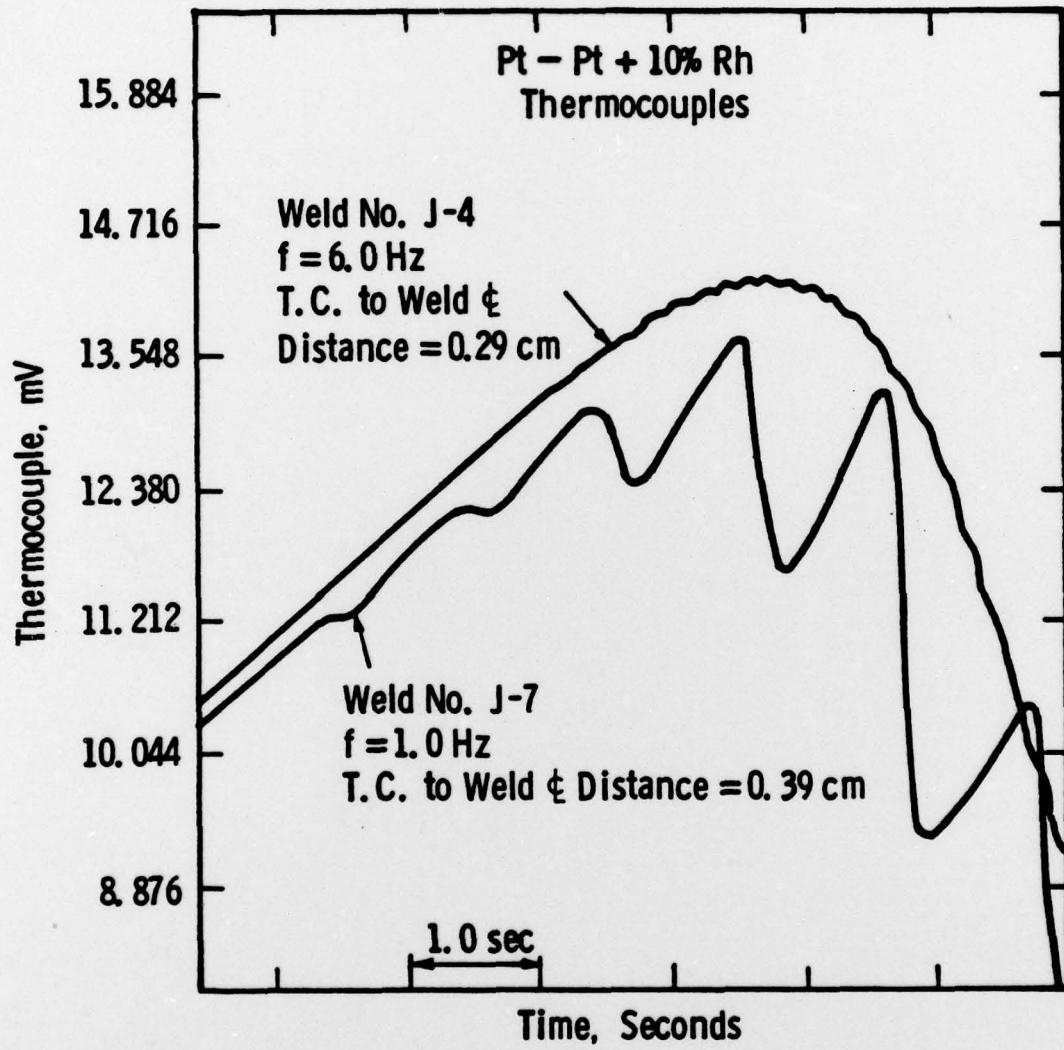


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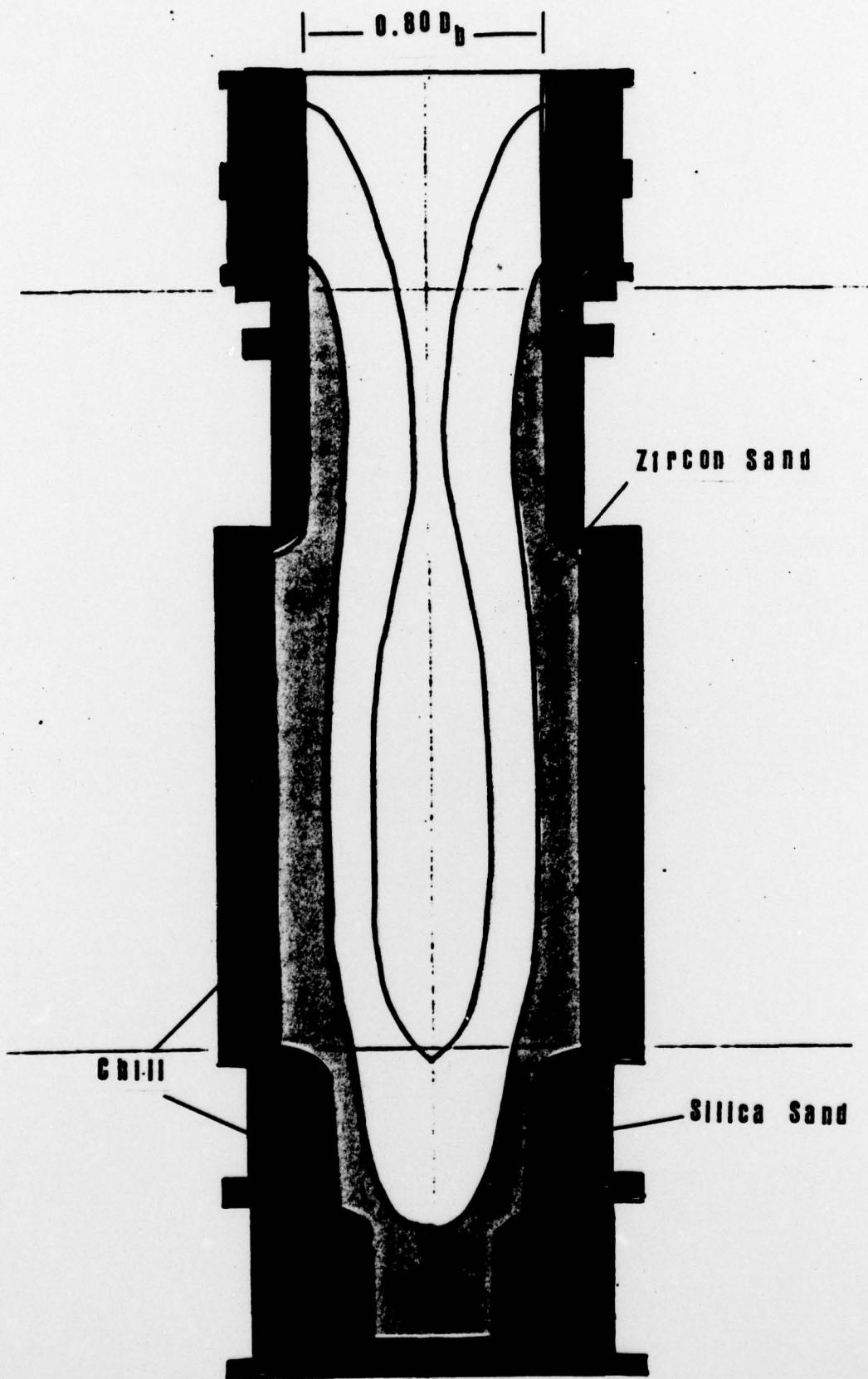


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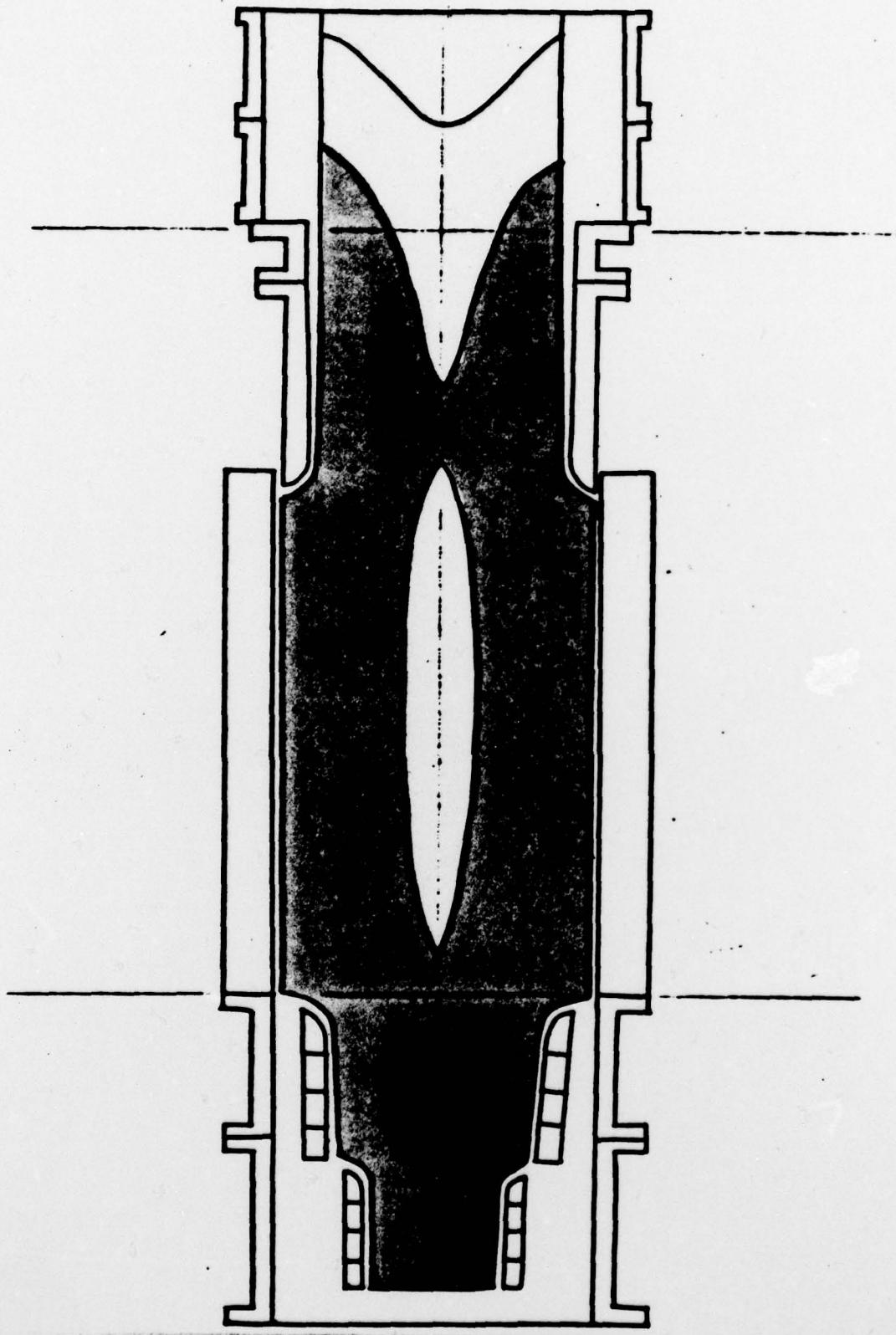


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4 IN/MIN: 692 DEG: 5 CM MOLD
—x— 16 CM DIA; — 38 CM DIA

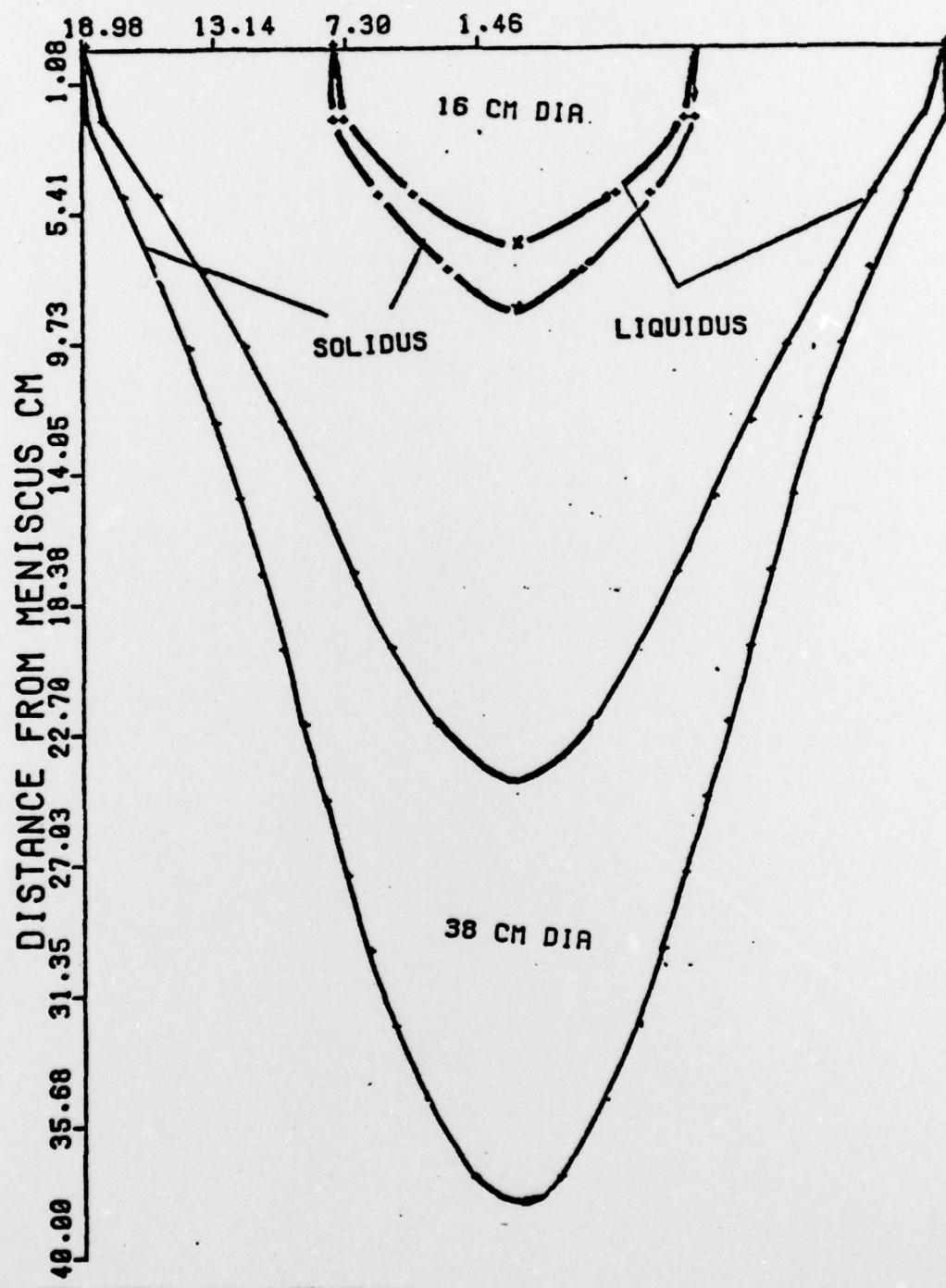


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Maximum normalized stress

1	1.801					
2	3.512	-0.233				
3	2.240	-0.103				
4	0.974	0.446	-0.434			
5	0.641	0.146	0.515			
6	0.534	0.468	-0.456			
7	0.464	0.814	-0.979	-0.647		
8	0.403	1.004	-1.294	-0.871		
9	0.340	1.001	0.062	-1.909	-1.610	
10	0.274	0.969	0.954	-3.137	-2.606	
11	0.208	0.906	1.304	-1.991	-4.635	-9.370
12	0.131	0.859	1.101	-0.414	-6.553	-7.820
13	0.089	0.767	1.050	0.731	-4.404	-9.265
14	0.078	0.659	1.030	1.480	-1.637	-8.439
15	0.080	0.676	0.990	2.389	0.729	-4.510
16	0.089	0.690	0.970	2.341	2.229	-0.517
17	0.097	0.688	0.985	1.870	3.465	2.122
18	0.101	1.668	1.012	1.655	2.661	3.304
19	0.098	0.631	1.056	1.541	2.138	1.186
20	0.087	0.581	1.084	1.513	1.947	1.876
21	0.072	0.529	1.092	1.562	1.896	1.802
22	0.073	0.486	1.097	1.625	1.975	1.893
23	0.070	0.466	1.114	1.684	2.118	2.081
24	0.056	0.462	1.152	1.757	2.258	2.320
25	0.055	0.469	1.209	1.848	2.402	2.558
26	0.070	0.485	1.275	1.952	2.546	2.779
27	0.101	0.514	1.335	2.049	2.684	2.976
28	-0.041	0.546	1.417	2.121	2.767	3.146

Axis of ingot

Bottom of ingot

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4 IN/MIN, 38 CM DIA, 5 CM MOLD
AL-MG ALLOY

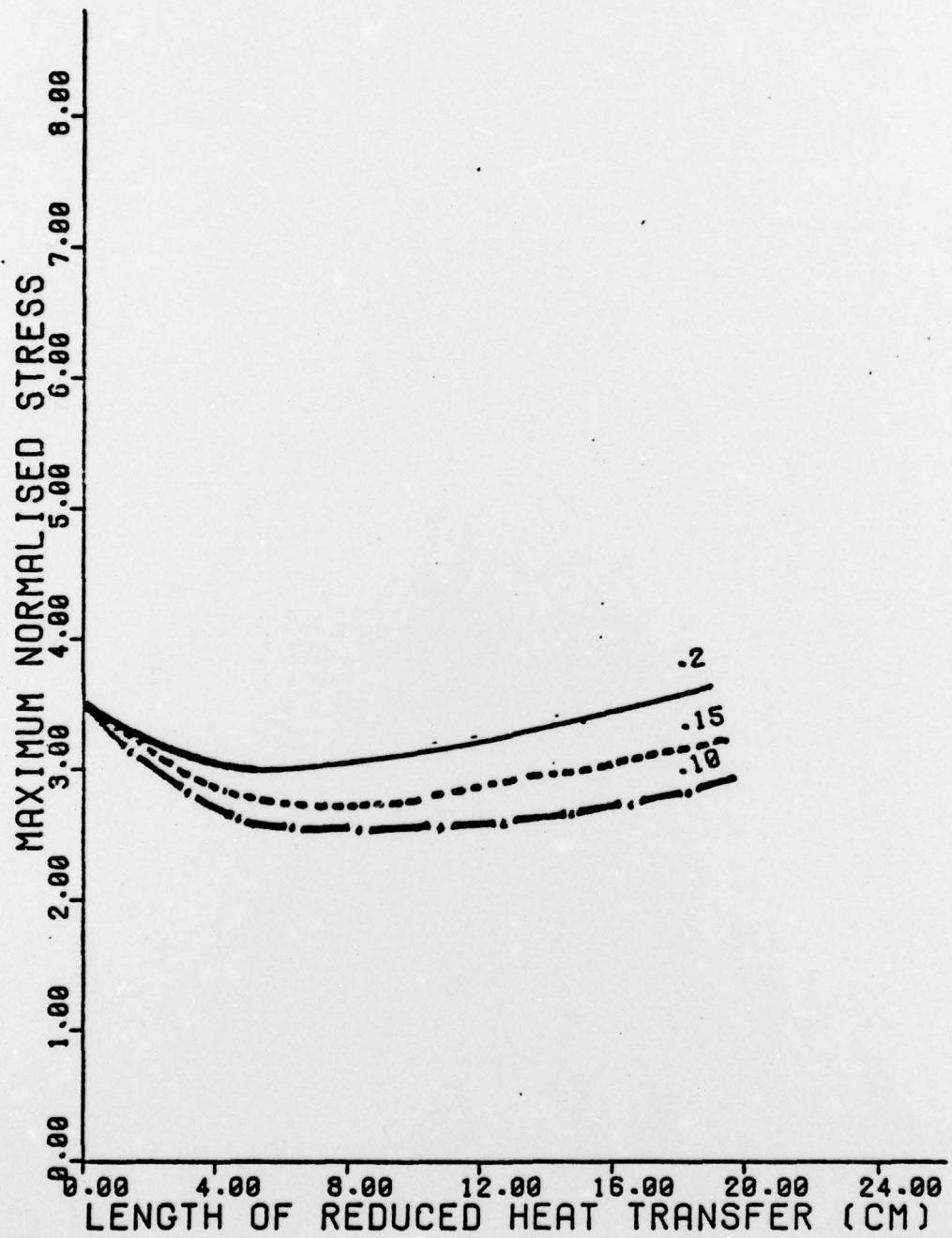


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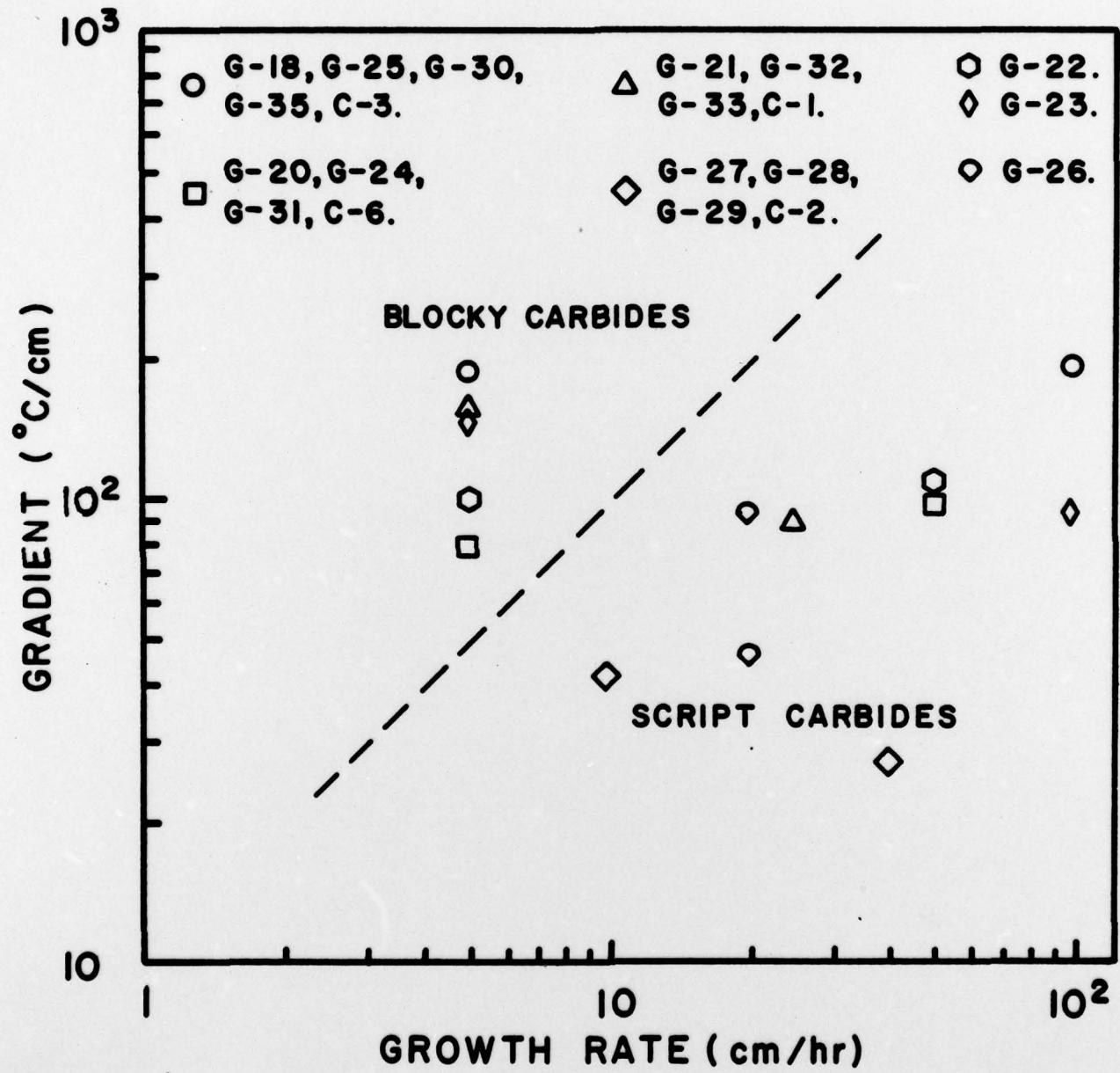


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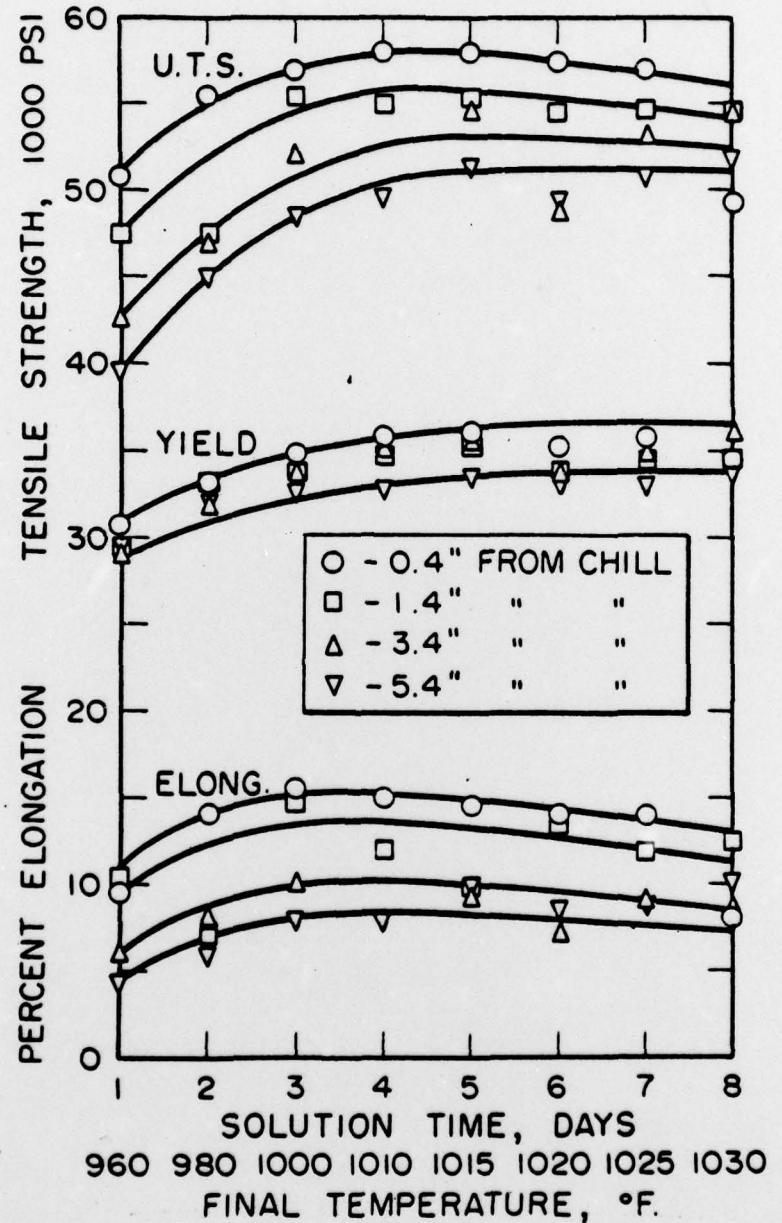


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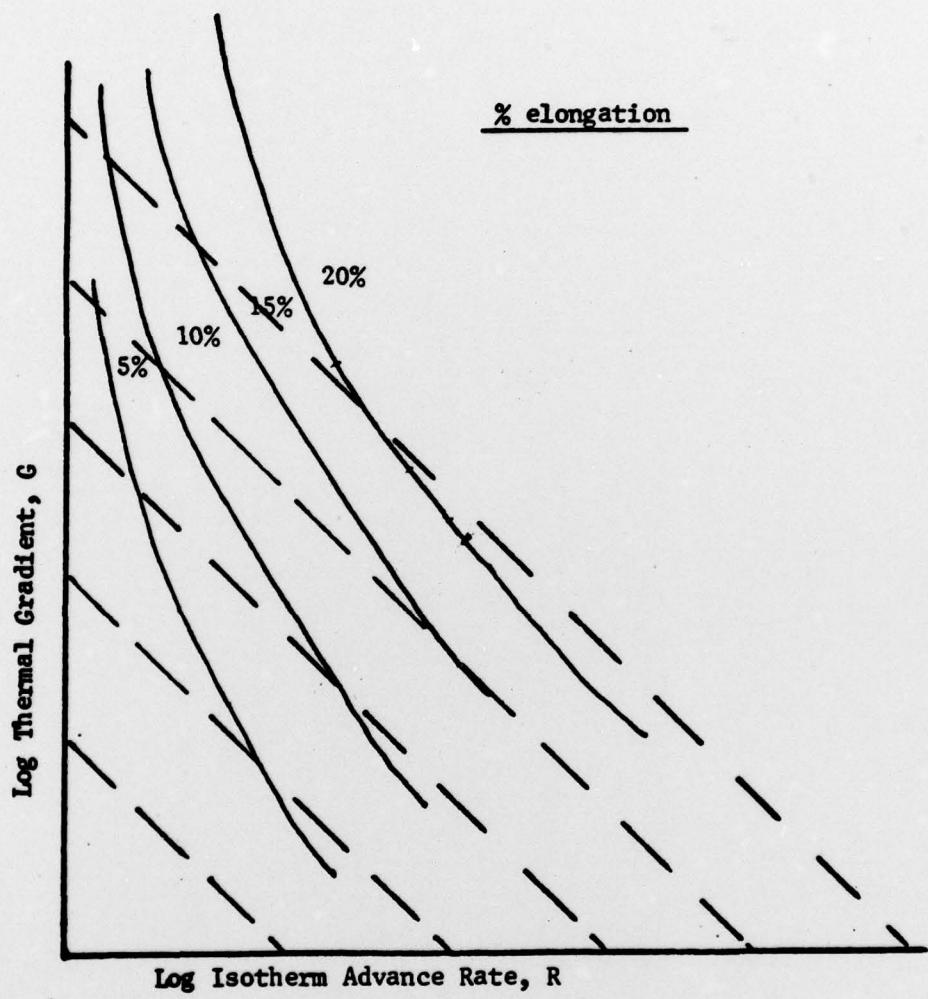


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